UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

DTIC FILE COPY (2)

REPORT DOCUMENTATION PAGE

AD-A219 557

1b. RESTRICTIVE MARKINGS

3. DISTRIBUTION / AVAILABILITY OF REPORT
Approved for public release; distribution unlimited.

4. PERFORMING ORGANIZATION REPORT NUMBER(S)
AFOSR-88

5. MONITORING ORGANIZATION REPORT NUMBER(S)
AFOSR-TR- 90-0306

6a. NAME OF PERFORMING ORGANIZATION
Inst. for Computational & Appl.
Univ. of Pittsburgh

6b. OFFICE SYMBOL (If applicable)

7a. NAME OF MONITORING ORGANIZATION
AFOSR/NM

6c. ADDRESS (City, State, and ZIP Code)
Pittsburgh, PA 15260

7b ADDRESS (City, State, and ZIP Code)
Bldg 410
Bolling AFB, DC 20332-6448

8a. NAME OF FUNDING / SPONSORING ORGANIZATION
AFOSR/NM

8b. OFFICE SYMBOL (If applicable)
NM

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
AFOSR-88-0262

8c. ADDRESS (City, State, and ZIP Code)
Bolling AFB, DC 20332

10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO
61102F	2304	A3	

11. TITLE (Include Security Classification)
Computational Fluid Dynamics

12. PERSONAL AUTHOR(S)
Charles A. Hall and Thomas A. Porsching

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 8/1/88 TO 11/30/89	90, 1, 31	

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Fluid Mechanics, Numerical Mathematics, Finite Element Methods, Navier-Stokes Equations, Divergence Free Subspace, Differential Algebraic Equations, Bifurcation Theory

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This research concerns projects of seven investigators at the University of Pittsburgh relating to the general area of computational fluid dynamics. Topics include the dual variable method, DAE's, the reduced basis method, divergence free finite elements, diffusive-transport systems, and bifurcation phenomena. Short descriptions of these projects are included, along with references to published reports.

Differential Algebraic Equations

DTIC ELECTE MAR 14 1990 S E D

20. DISTRIBUTION / AVAILABILITY OF ABSTRACT
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☐ DTIC USERS

21 ABSTRACT SECURITY CLASSIFICATION
Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL
Dr. Arje Nachman

22b TELEPHONE (Include Area Code)
(202) 767-4939

22c. OFFICE SYMBOL
NM

DD FORM 1473, 84 MAR

83 APR edition may be used until exhausted.
All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE

Final Technical Report

Air Force Office of Scientific Research Grant AFOSR-88-0262

Period: 1 August 1988 to 30 November 1989

Title: Computational Fluid Dynamics

Principal Investigators: C. A. Hall and T. A. Porsching

Institute for Computational Mathematics and Applications

Department of Mathematics and Statistics

University of Pittsburgh

Pittsburgh, PA 15260

January, 1990

Table of Contents

I. ACCOMPLISHMENTS

The following is a brief summary of the research accomplishments funded by AFOSR-88-0262, a grant to seven researchers of the Institute for Computational Mathematics and Applications, University of Pittsburgh.

1. Additive Correction Methods.

Using a general theorem that gives a bound on the iteration error in terms of an approximation error for the subspace containing the additive correction, realistic mesh independent contraction numbers have been derived for the convergence of a model two grid method. A second result shows that if the subspaces are chosen to be certain Krylov subspaces related to pseudo-residual vectors produced by the iterations, then the method is exactly a restarted preconditioned conjugate gradient method in which the splitting matrix plays the role of the preconditioner. Thus, the additive correction methods include this important class of iterative methods as a special case.

Regarding the convergence of generic iterative methods employing an additive correction phase, it has been shown [1] that if the coefficient matrix is symmetric, positive definite (SPD), if each additive correction step uses orthogonal projection with respect to the "energy" inner product, and if the range of each projector contains the most recent residual vector, then a contraction number for the error is $(\kappa - 1)/(\kappa + 1)$, where κ is the spectral condition number of the system. Thus, such methods are necessarily convergent. This work has recently been generalized [2] to the case where the coefficient matrix is only positive real; i.e., its symmetric part is SPD. The analysis in [2] is also general enough to yield contraction numbers for restarted versions of the ORTHOMIN and GCW generalized conjugate gradient methods described in [3].

It appears possible to sharpen the contraction numbers obtained in [1] and [2] by incorporating more information on the range of the projectors. This leads to the notion of abstract angles in projection methods.

References

[1] Chou, S. H. and Porsching, T. A., "A Note on Contraction Numbers for Additive Correction Methods", *Appl. Math. Lett.* 2 (1989), 83-86.

[2] Chou, S. H. and Porsching, T. A., "Contraction Numbers for Additive Correction Methods", to appear *Lin. Alg. and its Appl.*.

[3] Hageman, L. A. and Young, D. M., *Applied Iterative Methods*, Academic Press, New York, 1981.

2. Iterative Solution to Navier-Stokes Difference Equations.

The time-dependent two-dimensional Navier-Stokes equations are used to model the evolution of the flow of a Newtonian fluid. Implicit finite difference equations on a MAC discretization grid are used to approximate the continuity, enthalpy and momentum equations. By time-lagging the pressure and velocity variables in the enthalpy equations, the discrete enthalpy equations are uncoupled from the continuity and momentum equations and solved separately. The coupled system of discrete momentum and continuity equations is then transformed into the dual variable system [1, 2, 3], which is one-third the size of the coupled system.

The dual variable system was shown to be solvable for all problems unless the time step chosen is one of a finite number of values. New conditions which guarantee the solvability of the system for all positive real values of the time step were derived.

Special iterative methods for solving the dual variable system were developed. These methods were shown to converge to the solution under a variety of conditions. Also techniques for accelerating these iterative methods were constructed. These special iterative methods require the solution, on each iteration, of a linear system whose structure resembles a discrete Laplace equation; special methods of handling this with a minimum of operations were investigated.

DUALIT is a computer code which solves the time-dependent two-dimensional Navier-Stokes problem. To solve the dual variable system, DUALIT uses the transformed Jacobi iterative method and accelerates convergence with a second-order Richardson method. The aforementioned discrete Laplace system is solved with reduced-system Richardson iteration accelerated by the conjugate gradient method [4]. A comparison of DUALIT with DUVAL, a commercial program which uses banded Gaussian elimination to solve the same system of equations, shows that the dual variable solver in DUALIT uses less computer memory and considerably less computer time to solve the same problems. In [7], a simulation of the flow of air along the exterior of an aircraft and into an opening in the fuselage is anlayzed numerically. Inside the cavity, there is a sensor which is treated as a blockage. In front of the opening in the fuselage is a ramp or spoiler which causes the jetstream of air to shoot up over the opening and reduces the amount of flow into the cavity.

The inlet velocities on the bottom of the region correspond to a free stream Mach number of .75 while

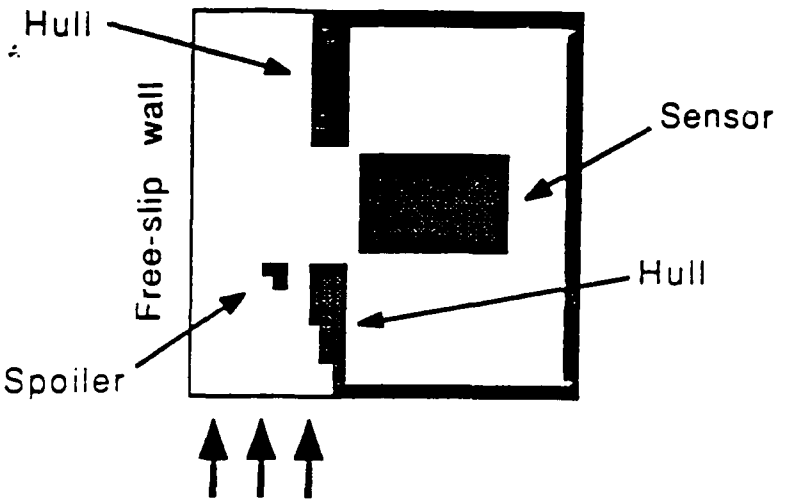

Figure 1. The Aircraft Cavity

pressures of 14.7 psi are specified at the outlet on the top of the region. The walls of the cavity and sensor are no-slip walls. The DUALIT code cannot handle walls on the interior of the region; therefore, the fuselage, spoiler, and sensor are approximated by adding large friction factors to the appropriate momentum equations to force the mass-velocities to be zero.

The solutions achieved by DUALIT and DUVAL agree to 2 significant places throughout the transient. Velocity magnitude contours are given in Figure 2 at time 25 seconds. From the figure one can see the effectiveness of using friction factors to simulate the interior blockages.

Figure 3 shows the streamlines of the flow at 25.0 seconds. As expected, the spoiler causes most of the air to stream up and over the opening. There is a small vortex just above and to the left of the sensor.

Figure 4 is representative of the gain in efficiency using the algorithm in DUALIT.

This research is contained in a Ph.D. thesis [5] of George Mesina, a student of Professor Charles Hall, and is also contained in a forthcoming joint paper [6].

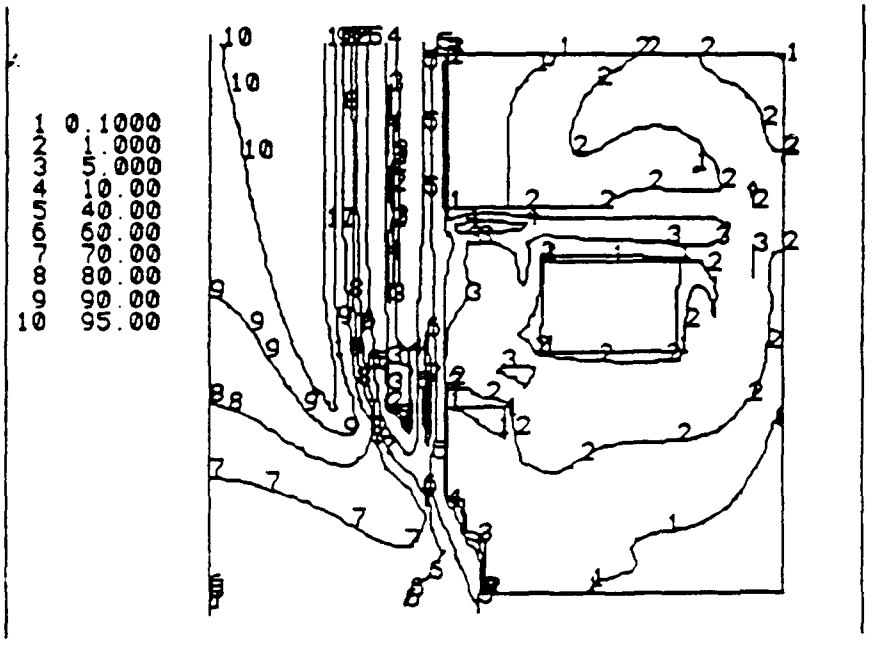

Figure 2. Aircraft Cavity Velocity Magnitude Contours at 25.0 Seconds

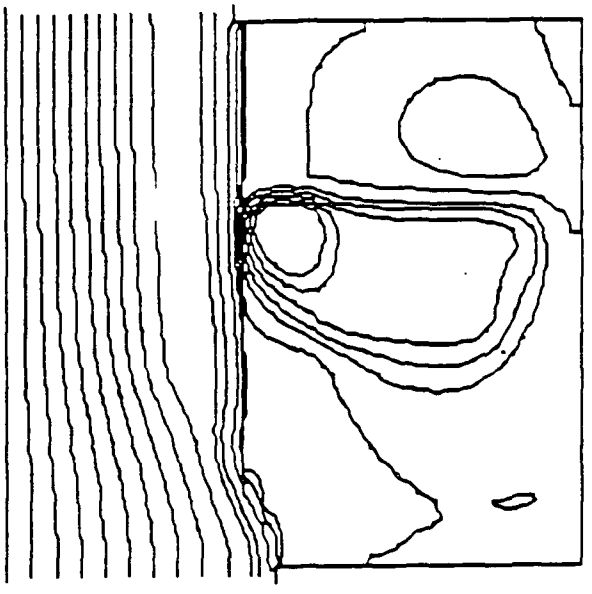

Figure 3. Aircraft Cavity Streamlines at 25.0 Seconds

We have developed an algorithm to construct cycle bases for MAC finite difference equations to extend the dual variable method [1, 2] to three dimensional analyses. This has been implemented on the CRAY/XMP.

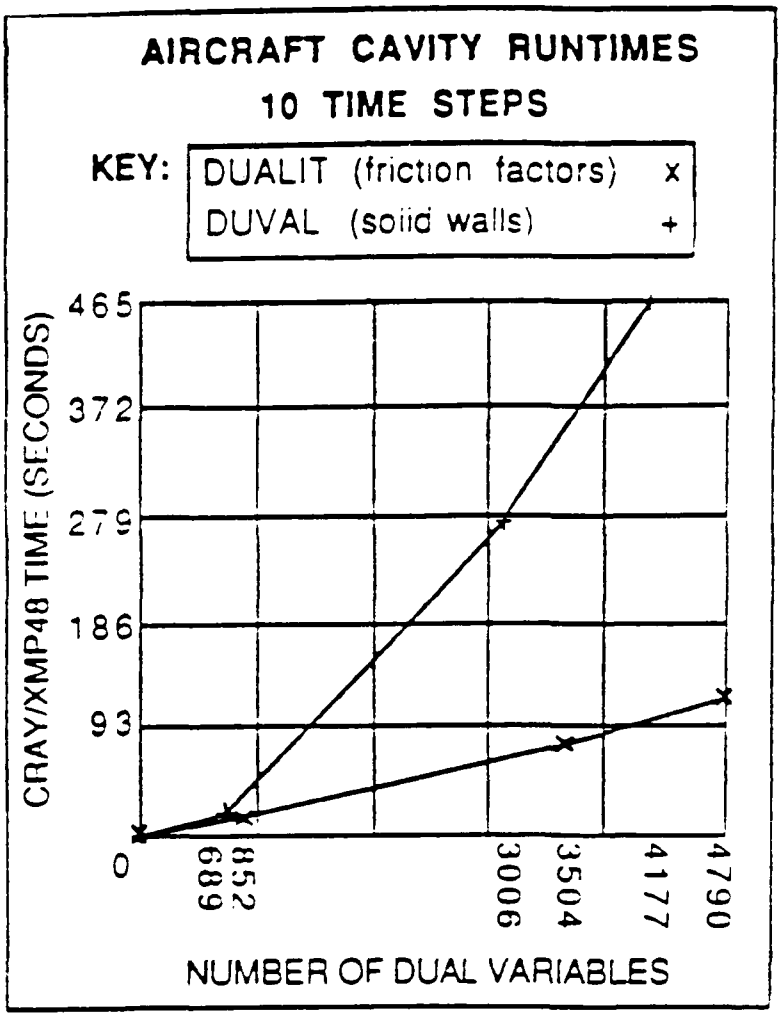

Figure 4. Comparison of Iterative and Direct Solvers on the CRAY/XMP48

An initial testing phase has been completed in which uniform flow, Poiseuille flow and driven cavity flows have been simulated successfully.

References

[1] Amit, R., Cullen, C. G., Hall, C. A., Mesina, G. L. and Porsching, T. A., "Flow Problems, Finite Differences, and the Frontal Method", *Third Int. Conf. on Flow Problems Proc.*, U. Calgary, 1980.

[2] Amit, R., Hall, C. A. and Porsching, T. A., "An Application of Network Theory to the Solution of Implicit Navier-Stokes Difference Equations", *J. of Comp. Phys.*, Vol. 40 No. 1, p. 183-201, 1981.

[3] Hall, C. A., Porsching, T. A. and Dougall, R. S., "Numerical Methods for Thermally Expandable Two-Phase Flow Computational Techniques for Steam Generator Modeling", *EPRI Report* NP-1416, Palo Alto, CA, 1982.

[4] Hageman, L. A. and Young, D. M., *Applied Iterative Methods*, Academic Press, Orlando, FL, 1981.

[5] Mesina, G. L., "Iterative Solutions to Navier-Stokes Difference Equations", Institute for Computational Mathematics and Applications Technical Report ICMA-88-122, University of Pittsburgh, 1988.

[6] Mesina, G. L. and Hall, C. A., "Iterative Solutions of Navier-Stokes Dual Variable Difference Equations", Institute for Computational Mathematics and Applications Technical Report ICMA-89-135, University of Pittsburgh, 1989. Submitted to *J. Comp. Phys.*

[7] Frey, A., Hall, C. A. and Porsching, T. A., "Numerical Simulation of Confined Unsteady Aerodynamical Flows", *Int. J. Num. Meth. Engr.*, 24, 1233-1250, 1987.

3. Solving Discrete Navier-Stokes Systems.

The focus of this project was solving the system of equations arising from discretizations of the incompressible Navier-Stokes equations in an efficient way. This remains one of the most challenging problems in computational fluid dynamics, with at least three basic issues:

(a) Linearization of the nonlinear system,

(b) Handling the incompressibility constraint,

(c) Finding an alternative less costly way to solve convection dominated diffusion equations than direct methods.

Our approach to dealing with these issues was to use a new iterative method based on conjugate gradient (cg) techniques. This was done with the aim of preserving the attractive features of cg, namely:

(i) Small storage requirements: $O(N)$ versus $O(N^{5/3})$ for efficient banded storage for direct methods needed to solve 2nd order partial differential equations in 3 space dimensions.

(ii) Low computational cost: $O(N^{4/3})$ versus $O(N^{7/3})$ for efficient banded elimination.

(iii) Ease of implementation: No parameters need to be supplied by the user, as for S.O.R. Also, it is not limited to simple geometry, as is multi-grid.

(iv) Convergence: cg iterates are theoretically proven to their error decreasing monotonically, and convergence is guaranteed within N iterations. (In practice, the iterations may be stopped on before N, since sufficient accuracy is obtained after only $O(N^{1/3}\log N^{1/3})$ iterations.

Unfortunately, the cg method was designed for linear symmetric systems of equations $Mx = b$. Thus it could not be applied to Navier Stokes discretizations, which are nonsymmetric nonlinear systems with additional

(incompressibility) constraints. Bi-conjugate gradients (*bcg*) is a generalization, designed for unsymmetric matrices. In describing how *bcg* arises from *cg*, we need to use a three-term recurrence relation satisfied by *cg* iterates x_k

$$x_{k+1} = \omega_k x_k + (1 - \omega_k)x_{k-1} + \omega_k \alpha_k r_k \ .$$

This is not the more standard description of *cg*, which is in terms of conjugate directions, as in [2]. It follows that the residuals $r_k = b - Mx_k$ also satisfy a similar relation:

$$r_{k+1} = \omega_k r_k + (1 - \omega_k)r_{k-1} - \omega_k \alpha_k M r_k \ .$$

Bcg introduces a new sequence of vectors defined to satisfy the residual relation for the transpose of the matrix:

$$S_{k+1} = \omega_k S_k + (1 - \omega_k)S_{k-1} - \omega_k \alpha_k M^T S_k \ .$$

The coefficients α_k and ω_k are defined as follows

$$\alpha_k = \frac{<S_k, r_k>}{<S_k, Mr_k>}$$

$$\frac{1}{\omega_k} = 1 - \frac{\alpha_k}{\alpha_{k-1}} \cdot \frac{<S_k, r_k>}{<S_{k-1}, r_{k-1}>} \cdot \frac{1}{\omega_{k-1}} \ .$$

Bcg preserves the (i) storage, (ii) computational cost, and (iii) algorithmic advantages of *cg*, but loses the theoretical convergence property (iv). In fact, the residual norms fluctuate quite drastically, making the method unusable. To remedy this, we introduce smoothing via an auxiliary sequence ρ_k of averaged residuals, which correspond to averaged solutions ξ_k.

The smoothing forces monotonic descent of residual norms, making *bcg* a usable method. The cost of implementing smoothing is negligable, the additional storage being 4 vectors, and the additional computations being 2 scalar multiplications of vectors and 2 dot products. Furthermore, the smoothing is only a "post-processing" operation, without interfering in any way with the *bcg* algorithm itself.

Bcg with smoothing is a computationally cheaper iterative method for nonsymmetric linear systems than others such as Orthonium [1], both in terms of op-counts and storage required. It constitutes one approach to issue (c) in the context of Navier-Stokes, We deal with issue (b) by actualy carrying out the *bcg* algorithm in

the space of solenoidal vector fields by means of projections. Issue (a) is the easiest to handle, via lagging. Substantial numerical computations with this new algorithm are reported in [3].

References

[1] H. Elman, Yale Univ. Report.

[2] D. G. Luenberger (1984): *Linear and Nonlinear Programming*, 2nd edition, Addison-Wesley, p. 244.

[3] S. Choudhury, "A Projected Bi-Conjugate Gradient Approach to Solving Discretized Incompresible Navier-Stokes Equations", ICMA Report.

4. Divergence Free Subspaces.

Finite element algorithms for solving the incompressible fluid flow problems must deal with the conservation of mass equations:

$$div\ q = 0 \tag{1}$$

where q is the mass velocity vector. Penality methods seem to be the popular approach, although other investigators have been able to construct special divergence free basis elements that satisfy (1) *a priori*.

Knowing such a basis, Galerkin's method involves a projection into this reduced subspace of divergence free velocity fields. Unfortunately, efforts in this direction up to now have involved straight sided elements and low order element approximation to the pressure.

The dual variable method, first introduced by Amit, Hall and Porsching [1], finds a basis for the null space of the discrete divergence operator using network theory. It was applied to the finite difference scheme proposed by Krzhivitski and Ladyzhenskaya [2] and a scheme using the discrete divergence and gradient operators of the MAC method studied by Harlow and Welch [3]. The DVM decouples the pressure from the velocity and results in a large reduction in the size of the linear system to be solved at each time step. Dougall, Hall and Porsching [4] implemented this method for finite difference discretization of Navier-Stokes equations used in the simulation of flow of thermally expandable steam water mixtures in reactor components.

Cha and Porsching [5] extended this method to finite difference discretizations of steady-state Navier-Stokes equations. Sledge [6] and Hall, Peterson, Porsching and Sledge [7] applied the DVM to finite element discretizations of transient Navier-Stokes equations. This work involved a 4-node quadrilateral element for

velocity and a constant quadrilateral element for pressure. No elements with curved edges were considered. Mansutti, et al [8] and Bulgarelli, et al [9] applied the dual variable method to two and three dimensional problems using finite difference approximations. Burkardt, Hall and Porsching [10] formulate a DVM for two dimensional compressible flow problems and Frey, Hall and Porsching [11] apply the DVM to analyze confined aerodynamical flows. Goodrich and Soh [12] interpreted the null basis in terms of the stream function for 2-D incompressible flow in driven cavities.

There have been many constructions of explicit bases of the divergence free subspace for various finite element and finite difference schemes. Griffiths [13, 14, 15] obtained an element level divergence free basis for several finite element schemes on triangular and quadrilateral elements. The techniques used are the same in each paper. Approximate values of the stream function at corner nodes are used to eliminate the unknown velocity components at midside nodes so that a typical divergence free function on each element is derived.

In Griffiths [13, 14], three types of finite element schemes were investigated on triangular elements which were given by Crouzeix and Raviart [16]. A divergence free basis was given for a nonconforming velocity field where the components of velocity are represented by piecewise linear functions defined in terms of their values at the midside nodes of the triangles. A divergence free basis also was given for a velocity field where the components of the velocity are piecewise quadratic functions defined in terms of values at the vertices and midside nodes of each triangle. The (discontinuous) piecewise constant pressure space was used for both of the above velocity spaces. Another divergence free subspace derived by Griffiths [13] involved a velocity field which comes from adding a cubic term to the quadratic representation. The pressure space used was a piecewise linear function with a single element support. Griffiths [15] derived a basis for the divergence free subspace of the 9-node biquadratic element velocity field on quadrilaterial elements. The following corresponding pressure spaces were investigated: constant, linear and bilinear elements. The basis functions for these pressure spaces have support on a single element. This allows the incompressible constraint to be analyzed one element at a time. But the basis function for the pressure space is discontinuous at element boundaries.

Gustafson, et al [17] combine group theory and fluid mechanics theory to obtain a basis for the divergence free subspace associated with the choice of quadratic velocity and constant pressure triangular elements in two dimension. Similar results have been obtained in 3-D for the scheme referred to as APX 3 in Teman [18]. The

late work by Gustufson, et al [19] can be viewed as augmenting and extending their previous work.

Stephens, et al [20] and Goodrich and Soh [12] applied the Galerkin finite difference method (GFDM) to the incompressible Navier-Stokes problem. This approach is similar to the Galerkin finite element method. The subspaces of discrete divergence free mesh vectors were constructed for several finite difference schemes. It is required that the discrete divergence and discrete gradient operators are formally adjoint. In Fortin [21], a subspace of S^h is constructed in which a function satisfies (1) for a subspace of the pressure space. This subspace is the orthogonal complement of piecewise constant pressure space. This can reduce the 5-node velocity and linear discontinuous pressure element to 4-node velocity and discontinuous constant pressure element.

We emphasize that all of the above constructions of divergence free basis velocity vectors require straight sided elements and that the pressure space contains only dicontinuous functions.

For many finite element and finite difference schemes, divergence free bases and null bases have been obtained. But most of them are for low order schemes and for very regular domains where the boundary is a piecewise straight line. In the current work a divergence free basis is constructed for a standard element type and curved edges are allowed.

Many numerical algorithms have been developed to solve this problem. Even though the null basis is not unique, we are interested in those which are sparse and banded. This means small support basis functions for the divergence free subspace and a banded sparse transformation matrix for the dual variable method.

The turn back algorithm is a method for computing a banded and sparse null basis. It was proposed by Topcu [22] to compute a null basis with a profile structure for equilibrium matrices in structural analysis. Kaneko, Lawo and Thierauf [23] interpreted this algorithm from a matrix factorization point of view. Berry, et al [24] refined this algorithm, implemented it using profile data structures and tested it on several structural problems. Berry and Plemmons [25] have implemented this algorithm on a HEP multiprocessor.

Coleman and Pothen [26] have designed two methods to obtain a sparse null basis: the first one computes a fundamental basis (one with an embedded identity matrix); the other one computes a triangular basis (one with an upper triangular matrix). Both algorithms have two phases. In the first combinatorial phase, a minimum dependent set of columns is identified by finding a match in the bipartite graph of the matrix. In the second, numerical phase, nonzero coefficients in the null vector are computed from this dependent set. Finding the

sparsest basis for the null space of an underdetermined matrix was shown to be NP-hard by Coleman and Pothen [27].

We have developed an algorithm which yields a basis for the divergence free subspace associated with the standard isoparametric 8-node velocity approximation and 4-node isoparametric pressure element. This basis has minimal support (no greater than 9 elements), can be efficiently constructed, and curved elements are allowed. The relation between this divergence free subspace approach and the dual variable method has been established. The turnback algorithm is used on a patch of elements. This work is contained in a forthcoming Ph.D. thesis of X. Ye, a Ph.D. student of Professor Charles Hall.

References

1. R. Amit, C. A. Hall and T. A. Porsching. (1981). An application of network theory to the solution of implicit Navier-Stokes difference equations. *J. Comp. Phys.*, 40, 183-201.
2. A. Krzhivitski and O. A. Ladyzhenskaya. (1966). The method of nets for the nonstationary Navier-Stokes equations, in Boundary Value Problems of Math. Phys., Amer. Math. Soc. Transl., *Proc. Math. Inst. Steklov*, 92.
3. F. H. Harlow and J. E. Welch. (1965). Numerical calculation of time dependent viscous incompressible flow of fluid with free surface. *Phys. Fluids.* 8, 2182-2189.
4. R. S. Dougall, C. A. Hall and T. A. Porsching (1982). DUVAL: A computer program for the numerical solution of two-dimensional, two-phase flow problems. *Vol. 1-3, EPRI. Report*, NP-2099, Palo Alto, CA.
5. A. Cha Lin and T. Porsching. (1982). On the Krzhivitski-Ladyzhenskaya difference method for the stationary Navier-Stokes equations. *Proc. 10th IMACS World Congress*, Montreal, Canada (R. Peskin Ed.).
6. F. Sledge. (1983). A finite element implementation of the dual variable method for the Navier-Stokes. *Ph.D. Dissertation*, Univ. of Pittsburgh, Pittsburgh, PA., and *Technical Report ICMA-83-60.*
7. C. A. Hall, J. Peterson, T. Porsching and F. Sledge. (1985). The dual variable method for finite element discretizations of Navier-Stokes equations. *J. Numer. Meth. In Eng.*, 21, 883.
8. D. Mansutti, U. Bulgarelli, R. Piva and G. Graziani. (1986). A discrete vector potential method for unsteady 3-D Navier-Stokes equations. *10th ICNMFM*, Beijing.
9. U. Bulgarelli, G. Graziani, D. Mansutti and R. Piva. (1986). A reduced implicit scheme, via discrete stream function generation, for unsteady Navier-Stokes equations in general curvilinear coordinates. *6th GAMMA Conference*, Gottingen, West Germany.
10. J. Burkardt, C. Hall and T. Porsching. (1986). The dual variable method for the solution of compressible fluid flow problems. *SIAM J. Alg. Disc. Meth.*, Vol. 7, No. 3.
11. A. Frey, C. Hall and T. Porsching. (1987). Numerical simuilation of confined unsteady aerodynamical flows. *Inter. J. Num. Meth. Eng.*, 24, 1233-1250.
12. J. W. Goodrich and W. Y. Soh. (1988). Time dependent viscous incompressible Navier-Stokes equations: The finite difference Galerkin formulations and stream function algorithms. *To appear in J. Comp. Physics.*
13. D. F. Griffiths. (1979a). Finite elements for incompressible flow. *Math. Meth. in Appl. Sci.*, 1, 16-31.
14. D. F. Griffiths. (1979b). The construction of approximately divergence-free finite element in *The Mathematics of Finite Element and Its Applications III*, Ed., J. R. Whitemen, Academic Press.

15. D. F. Griffiths. (1981). An approximately divergence-free 9-node velocity element for incompressible flows. *Inter. J. Num. Meth. in Fluid.*

16. M. Crouzeix and P. A. Raviart. (1973). Conforming and nonconforming finite element methods for solving the stationary Stokes equations I. *R.A.I.R.O.*, R-3, 33-76.

17. K. Gustafson and R. Hartman. (1983). Divergence-free basis for finite element schemes in hydrodynamics. *SIAM J. Numer. Anal.*, 20, 697-721.

18. R. Teman. (1977). *Navier-Stokes Equations: Theory and Numerical Analysis.* North-Holland, Amsterdam.

19. K. Gustafson and R. Hartman. (1985). Graph theory and fluid dynamics. *SIAM J. Alg. Disc. Methd.*, Vol. 6, No. 4.

20. A. B. Stephens, J. B. Bell, J. M. Solomon and L. B. Hackerman. (1984). A finite difference Galerkin formulation for the incompressible Navier-Stokes equations. *J. Comp. Physics*, 53, 152-172.

21. M. Fortin and A. Fortin. (1985). Experiments with several elements for viscous incompressible flows. *Int. J. Num. Meth. Fluid*, 5, 911-928.

22. A. Topcu. (1979). A contribution to the systematic analysis of finite element structures through the force method. *Ph.D. Thesis*, Univ. of Essen, Essen, Germany.

23. I. Kaneko, M. Lawo and G. Theirauf. (1982). On computational procedure for the force method. *Inter. J. Num. Meth. in Eng.*, 19, 1469-1495.

24. M. Berry and M. Heath, I. Kaneko, M. Lawo, R. Plemmons and R. Ward. (1985). An algorithm to compute a sparse basis of the null space. *Numer. Math.*, 47, 483-504.

25. M. Berry and R. Plemmons. (1985). Computing a banded basis of the null space on the Denelcor HEP multiprocessor. *Proc. AMS/SIAM Summer Conf. on Linear Algebra in System Theory*, AMS Series on Contemp. Math.

26. T. Coleman and A. Pothen. (1987b). The null space problem II: Algorithms. *SIAM J. Alg. Disc. Math.*, 8, 544-563.

27. T. Coleman and A. Pothen. (1987a). The null space problem I; Complexity. *SIAM J. Alg. Disc. Meth.*, 7, 527-537.

5. Numerical Solution of Transport, Slightly Diffusive Transport and Fluid Flow Problems.

A central theme of this project has been the numerical analysis of multidimensional transport and slightly diffusive transport problems. The research can be broadly divided into the following (closely interrelated) areas:

a. Classification, comparison and parameter selection for difference schemes for 2-D convection-diffusion problems.

b. Derivation of monotone type discretizations for boundary value problems.

c. Numerical analysis of defect or deferred correction methods for multi-dimensional convection diffusion equations.

d. Numerical and analytical studies of natural convection problems.

a. Classification of schemes for 2-D convection diffusion problems

In Layton [1], structure has been given to the many schemes proposed for 2-D convection-diffusion problems via the theory of modified equations. One desirable feature in a numerical methods for convection-diffusion problems is that artificial diffusion operate primarily in the streamline direction. In the preliminary study [2] it was pointed out that with positive type stencils for general (a, b) the amount of "crosswind" smearing due to artificial viscosity must be substantial in a quantifiable manner. This idea was more fully developed (for general stencils) in Layton [1].

As a concrete example of the generally applicable theory of Layton [1], consider the celebrated "skew-upwind" scheme (proposed by Raithby in 1976) which was a precursor of the currently popular streamline diffusion methods. In [1] it was shown that the principal axes of diffusion of this scheme are not aligned with the streamline direction unless (a, b) is aligned with the mesh [$a = 0$, $b = 0$ or $a = b$]. Futher, in [1, example 4] it is shown how the skew upwind scheme should be "realigned". The resulting scheme is, in fact, of *positive type* while the skew-upwind scheme is not! Numerical experiments in [1, section 4] confirm the superiority of this new scheme over both the original skew-upwind method and other positive-type upwinding formulas.

b. Derivation of Monotone Type Discretizations for Boundary Value Problems

The well-known stability barrier of van Veldhuizen states that for general velocity fields (a, b) a positive type approximation of L_ε in (1) is limited to first order accuracy. In Layton [1] it was shown that, even among first order schemes, for general (a, b) positive type stencils must possess substantial cross-wind diffusion in a quantifiable sense. Thus, there is also a barrier in the spurious cross-wind diffusion in these schemes. Further, for second order elliptic equations with cross-derivative (u_{xy}) term there is also a stability barrier (due to Greenspan and Jain) on the size of the u_{xy} coefficient for the existence of positive type discretizations, (see Layton [14] for a more complete discussion).

Thus, the sign pattern required of positive type stencils is clearly too restrictive for accuracy. On the other hand, it is very desirable to have discretizations which satisfy a discrete maximum principle/preserve positivity. Thus, schemes which lead to monotone type (or inverse positive) discretization matrices must be considered.

This condition on the stencil is global. One contribution of this research is that it has been shown how to

correctly "microlocalize" this condition.

A general methodology for the microlocal construction, which is based upon the theory of regular splittings was derived and analyzed in Layton [15]. To describe it, we shall focus on the convection-diffusion problem (1). Consider first the case $\varepsilon = 0$, (we will return to the $0 < \varepsilon$ "small" case soon). One basic problem is going from the microlocal problem (pre-monotone stencils) to the global problem (variable coefficient problems). Loosely speaking, this difficulty arises because matrix multiplication is row by column, thus, a point-by-point splitting of L_ε^h into "generalized positive type decompositions" will not induce a matrix splitting when boundaries or variable coefficients are present. Two principles of "microlocalization" have been proposed which resolve this difficulty. The first method, in Layton [15], is based upon a novel theory of difference schemes, intermediate between positive type and general monotone type schemes, Positive Averaged Stencils (PAS). These were introduced in Layton [14] where the relevant theory is developed.

Thus, positive averaged stencils are one way to pass from local constructions of L^h to global conditions on $(L^h)^{-1}$! Interestingly, all of the classical monotone type discretizations of second order problems are positive averaged stencils, with one exception in Layton and Morley [17]. The extra degrees of freedom in PAS and relaxation of the sign pattern can be used, for example, to increase the accuracy in methods.

The treatment of boundary conditions inside the P.A.S. framework is not difficult. To preserve monotonicity in the non-periodic case we use, at the points adjacent to the boundary, a lower order discretization. This discretization is determined by computing the operator splitting $P^h \cdot A^h$ restricted to those points. In this fashion we generate one "compatible" with the interior equations.

To analyze the singularly perturbed case a "collage" type result was proven in Layton [15] monotone (or inverse positive) matrices. The "collage lemma" of Layton [15] gives a result which has a degree of uniformity in the dimension of the matrices involved.

The second principle of microlocalization was presented in Layton [14]. It involves differencing variable coefficient problems, not via the frozen coefficient problems at each point, but rather selectively values of the coefficients at the meshpoint as well as its nearest neighbors. This procedure is quite general and systematic. The derivation of the variable coefficient stencil can be summarized as follows:

Suppose, in the constant coefficient case a stencil L^h possesses a "generalized positive type decomposition" (in the sense introduced by Brandt), specifically

$$\begin{cases} L^h = \Lambda^+ \cdot \Lambda^- - R \ , \ R \geq 0 \ \text{coefficientwise} \ , \\ \Lambda^+ \ , \ \Lambda^- \ \text{are positive type difference stencils} \ . \end{cases}$$

Then, the correct extension of L^h to variable coefficient problems is in terms of the frozen coefficient problems in Λ^+ and Λ^- rather than in L^h!

In summary, progress on monotone type discretizations has been substantial. The question of derivation of stencils of the required type has been substantially solved and promising work is underway on the remaining issue (2-D convection-diffusion). The "micro-localization" question is completely resolved in its full generality. Treatment of points adjacent to computational boundaries has been successfully addressed in several examples by ad-hoc methods. Additive combination of monotone type stencils with positive type stencils has been resolved in the case of a "small" perturbation in the collage lemma.

c. Numerical Analysis of Deferred Correction Methods

A promising algorithm for multidimensional convection problems, originally due to Hemker [6], based on deferred corrections was analyzed in Ervin and Layton [3] and Axelsson and Layton [4], [5] and [18]. Additional work included extensive numerical experiments, reported in Ervin and Layton [13] and research code, documented in Ervin and Layton [16]. In spite of intensive computational studies of (DCM), rigorous error analysis was lacking for problems with realistic boundary layers.

In Ervin and Layton [3], a finite difference implementation of (DCM) was analyzed for the two-point B.V.P. arising as the 1-D version of (1). In this case, uniform in ε (singular perturbation parameter) convergence of optimal orders on subdomains was proven. Precise estimates near layers were given in [3] also.

These estimates were also proven to be sharp in numerical experiments reported in Ervin and Layton [3]. The local error analysis via cutoff functions was carried out for the 2-D problem in Axelsson and Layton [4]. This analysis focused on a finite element interpretation of (DCM). To summarize the basic result, let Ω_j be a nested sequence of subdomains.

$$\Omega \supset \Omega_1 \supset \Omega_2 \supset \cdots \supset \Omega_J \ , \tag{3}$$

such that each Ω_j does not admit upstream cutoff, as pictured Figure 1. Further, suppose

(i) the characteristic portion of $\partial\Omega_j$ is $0(\sqrt{h}\ ln(1/h))$ distance from $\partial\Omega_{j-1}$,

(ii) the outflow portion of $\partial\Omega_j$ is $0(h\ ln(1/h))$ distance from $\partial\Omega_{j-1}$,

(see [4] for a precise formulation), where h is the maximum diameter of the finite element triangulation of Ω. The basic result in Axelsson and Layton [4] states that when the finite element space approximates smooth functions to $0(h^k)$ in $H^1(\Omega)$, the error $u - U^j$ is of optimal order, uniformly in ε on subdomains, modulo a term which is of infinite order accuracy, nonuniformly in ε.

Theorem Let $u :=$ true solution of (1), $U^j := j^{th}$ finite element, defect correction approximation, then for any $s > 0$,

$$\|u - U^j\|_{H^1(\Omega_j)} \leq C_1(f, s)\{(\varepsilon_0 - \varepsilon)^j + h^k\} + C_2(\varepsilon)\varepsilon_0^s .$$

d. Numerical and Analytical Studies of Natural Convection Problems

Convection-diffusion equations are useful *models* of more complex physical processes, such as coupled Navier-Stokes system in free or natural convection problems, studied in Boland and Layton [7], [8], [12] and Ermentrout, Boland, Hall, Layton and Melhem [9]. In this work, a finite element model of natural convection in an enclosure with thermally conducting walls is studied, based upon a Boussinesq model.

In a preliminary study, the stability and regularity properties of the Boussinesq model (4) was analyzed. This study includes the discontinuous coefficient κ and the coupling between the energy and the Navier-Stokes equations. This preliminary study elucidates expected regularity properties of the solution $(\underline{u}, p, T)$ of (4). With this knowledge in hand, in Boland and Layton [7], the finite element method for the time dependent coupled system was analyzed. Error estimates were proven for the time dependent problem. These estimates delineate both expected convergence rates under minimal data restrictions as well dependence of the error upon the Prandtl and Rayleigh (Pr, Ra) numbers.

In a companion analysis [12] (incorporating the report [8]), we consider the steady state problem. Error estimates, under global and local uniqueness conditions, are proven for the finite element model. The assumptions on the continuous problem are also proven in a separate section of [12]. One interesting auxiliary result

proven in Boland and Layton [19] is as follows. Consider the steady state problem arising before subtracting of the boundary conditions specifically $\gamma = 0$ with inhomogeneous Dirichlet boundary conditions on $\partial_2\Omega$ in (4). It was shown in [12] that the continuous problem always has at least one steady state solution, which is unique for small data and generically, locally unique for large data. The corresponding question can be asked for the finite element model: does the finite element model admit steady state solution?

Case 1: $dist(\partial\Omega_e, \partial\Omega) > 0$. The answer here is yes.

Case 2: Linear or bilinear elements plus an angle or aspect ratio condition. The answer here is yes, via a discrete maximum principle argument in the energy equation.

Case 3: Quadratic or higher elements for the temperature. In this case the following condition is needed to ensure a yes answer: either $dist(\partial\Omega, \partial\Omega_e) > 0$ or $\Omega = \Omega_e$ and: the local mesh density near the vertical sides of $\partial\Omega_e$ must be sufficiently small, in a quantifiable sense, depending on Pr and Ra : $h_{\text{loc}} = C\ Ra^{-1/4}$ near $\partial\Omega_e$. This result is in accordance with the engineering practice of grading the mesh near $\partial\Omega_e$ as in (5). In fact, a formal asymptotic analysis of layers in (9) suggests that the boundary layers are in fact within $0(Ra^{-1/4})$ of $\partial\Omega_e$.

This idea was developed in a different direction in [9]. It is well known that discretizations of nonlinear problems frequently introduce spurious solutions. In, e.g., Stephens and Shubin [10], it was shown how these spurious steady state solutions are introduced for Burger's equation, by spatial discretization. Motivated by non-physical dynamics observed in the finite element model of hollow glass blocks, in [9], we study how these non-physical steady states influence the *dynamics* of the *time dependent* Burger's equation. In some cases, we have rigorously proven that a Hopf bifurcation does occur in the discrete system. This is consistent with the computational results reported in Melhem [11].

References

[1] Layton, W., "On the principal axes of diffusion in difference schemes for 2-D transport problems", I.C.M.A. Report 88-124, *J. Comp. Phys.* to appear.

[2] Layton, W., "On crosswind diffusion in difference schemes", I.C.M.A. Report 87-111, (this note is now incorporated into reference [1] and submitted to *J. Comp. Phys.).*

[3] Ervin, V. and Layton, W., "A study of defect-correction, finite difference methods for convection diffusion equations", *SIAM J.N.A. (1988).*

[4] Axelsson, O. and Layton, W., "Optimal interior estimates for the defect correction, finite element approach to 2-D convection diffusion problems", I.C.M.A. Report 88-116, incorporated into [5].

[5] Axelsson, O. and Layton, W., "Defect correction methods for convection dominated, convection diffusion equations", to appear in: *R.A.I.R.O., J. Num. Anal.* (now *M.A.N.)*

[6] Hemker, P. W., "An accurate method without directional bias for the numerical solution of a 2-D singular perturbation problem", in: *Thy. and Appls. of Sing. Pert.*, (W. Eckhaus and E. M. de Jaeger, eds.) Springer LNM, vol. 942, Springer Berlin, 1982.

[7] Boland, J. and Layton, W., "An analysis of the finite element method for natural convection problems", I.C.M.A. Report number 88-126, *Numerical Methods for P.D.E.'s.*, to appear.

[8] Boland, J. and Layton, W., "On the "determining modes" question for nonlinear operator equations", I.C.M.A. Report 88-119, incorporated into [12].

[9] "Analytical and numerical studies of natural convection", Boland, J., Ermentrout, G.B., Hall, C.A. and Melhem, H., I.C.M.A. Report 88- , to appear in: *Proc. Int. Conf. on Thy. and Appls. of Diff. Eqns.*, 1988.

[10] Stephens, A. B. and Shubin, G. R., "Multiple solutions and bifurcation of finite difference approximations to some steady problems of fluid dynamics", *SIAM J.S.S.C.*, 2(1981) pp. 404-415.

[11] Melhem, H., "Finite element approximation to heat transfer through combined solid and fluid media", Institute for Computational Mathematics and Applications Technical Report, ICMA-87-107, 1987 (MS Thesis).

[12] Boland, J. and Layton, W., "On finite element approximation of steady natural convection problems," submitted. 1989.

[13] Ervin, V. and Layton, W., "High resolution, minimal storage algorithms for convection dominated, convection-diffusion equations," A.R.O. report 87-1, pp. 1173-1201 in: *Trans. of the Fourth Army Conf. on Appl. Math. and Computing, 1987.*

[14] Layton, W., "A novel, monotone-type difference scheme for general second order elliptic equations," K.U.N. Report, June 1989, submitted currenty under review.

[15] Layton, W., "On the construction of monotone type discretizations for boundary value problems for partial differential equations," K.U.N. Report. June 1989, submitted for publication.

[16] Ervin, V. and Layton, W., "A modified defect-correction algorithm for the solution of singularly perturbed differential equations," documentation for the research code DEFCOR.

[17] Layton, W. and Morley, T. D., "On central difference approximations to general second order elliptic equations," *Lin. Alg. Appls.*, 97 (1987), 65-75.

[18] Axelsson, O. and Layton, W., Iterative Methods as Discretization Procedures, to appear in: *Proc. Int. Conf. on P.C.G. and Appls.*, 1989.

[19] Boland, J. and Layton, W., in preparation.

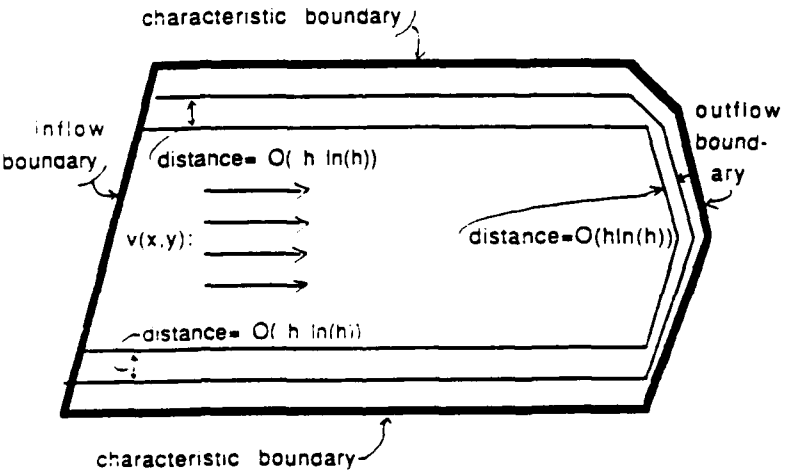

Figure 1

6. Equilibrium Manifolds in Computational Mechanics

Throughout the past several years, one aspect of our research program concerned the computational solution of equilibrium problems as they arise naturally in continuum and fluid mechanics. The mathematical models for describing these problems are formed by nonlinear equations, including algebraic, differential, or integral equations, all of which involve several parameters, and hence have the generic form $F(z,\lambda) = 0$. Here z varies in some space Z and characterizes the state of the physical system while λ denotes the vector of parameters from some finite dimensional space Λ.

Our research in this area has been based on a consistent use of the fact that the solution set of such parametrized equations constitute in general, a differentiable manifold in the product space $X = Z \times \Lambda$. Our results so far certainly show the value and power of this geometric approach.

Our work concerns essentially the following topics:

(1) Development of methods for analyzing various features of equilibrium manifolds on the basis of a computed simplicial approximation.

(2) Methods for the computation of sub-manifolds of foldpoints on equilibrium manifold.

(3) Study of estimation techniques for the errors arising in the various computational procedures under (1) and (2).

Some details of the current work are given in the following sub-sections.

i. *Methods for Analyzing Features of Equilibrium Manifolds.*

A new method for computing simplicial approximation of the solution manifolds of a parametrized equation has been developed. An essential part of the method is a constructive algorithm for computing moving frames; that is, of orthonormal bases of the tangent spaces that vary smoothly with their points of contact. The approximation process uses these bases together with a chord form of the Gauss-Newton method as a corrector, to compute the desired nodes of the simplicial mesh on the manifold.

The process has been implemented for two-dimensional as well as three-dimensional manifolds in spaces of arbitrary dimension. All experience with these codes so far has been excellent. In particular, it turns out that the method is extremely efficient and in fact has a better computational complexity than most continuation procedures. For example, for a two-dimensional manifold a typical computation produces a triangulation involving 114 triangles with 19 evaluations and decompositions of the Jacobian of the mapping. Work is continuing on the process. In particular, we are currently experimenting with adaptive approaches for handling situations involving large changes of the curvature of the manifold.

Any simplicial approximation computed with this method provides a wealth of information about the equilibrium manifold. This opens up numerous possibilities for determining various features of such manifolds.

A first possibility is of course to provide a graphical representation of parts of the manifold. Such an opportunity has not existed before and already simple examples indicate what new insight can be obtained in this way. At the same time, effective graphics techniques for visualizing a p-dimensional manifold defined in a high dimensional space are by no means readily available. During the past year a set of post-processing routines have been developed which generate a sequence of slices of a simplicial approximation of a three-dimensional manifold. Suitable projections of these two-dimensional slices can then be represented graphically by means of standard programs, such as MOVIE.BYU. By viewing these slices in sequence one has the impression of "flying" through the 3-dimensional manifold and this provides often some unique insight into its features. Work is now continuing to incorporate plots of prescribed contour surfaces into these graphical representations.

Graphical representations are, of course, only one way to analyze the various features of our manifolds. The wealth of computed data offer numerous possibilities for the application of post-processing routines to calculate approximations of various specific features.

A particularly important feature is the curvature tensor of the manifold M which has many important applications. The numerical calculation of the curvature tensor from the data made available by the moving frame algorithm was set as one of the goals of the previous proposal. The differential geometric and numerical difficulties, the latter being essentially due to the fact that curvature depends upon second-order quantities, have been successfully overcome in [1]. The corresponding algorithm has provided surprisingly good results. Moreover, an unexpected by-product of this method was found in the form of the apparently first efficient and

rigorous technique for the calculation of all the bifurcated branches of solutions in bifurcation problems involving a higher dimensional null-space. Up to now, only the one-dimensional null-space case had been considered (and so, extensively) in the numerical literature.

As noted earlier the availability of some approximation of the curvature tensor has many important applications. One of them concerns the question of estimating the distance from a given point x on M to some foldpoint x* of that manifold. As part of the methods for computing foldpoints discussed in the next subsection we have developed a method for obtaining such estimates. In essence, a foldpoint on M is defined by the property that one or several normal vectors of M at that point are parallel to the given natural parameter space Λ. This suggests the computation of the smallest principal angle between the (n-p)-dimensional normal space rgeDF(x)* and the p-dimensional natural parameter space Λ. These principal angles are readily computed, but, of course, without any further information they do not provide the desired estimate of $\|x-x^*\|$. Here the approximate curvature tensor can be used very effectively. This provides, for the first time, a computable estimate for this important distance. Results so far with the technique are very encouraging but further work is needed to make the method generally applicable.

The computed simplicial approximations also provide an effective tool for determining the approximate location of the foldset of the manifold M. For this one has to monitor the orientation of the projection of the tangent basis at the nodal points onto the parameter space Λ. If there is a change in this orientation then we are in the neighborhood of a foldpoint; but the converse is not necessarily true, since not every foldpoint can be detected this way. The orientation can be characterized, for example, by the determinant of the projected basis in the parameter space. Thus, in essence, if we plot lines of constant determinant values, then lines of zero determinant values are approximations of the desired foldlines. Of course, determinants are not always the best way to proceed here, and we are currently studying alternate techniques for the effective determination of the desired orientation changes and for combining the technique with the above mentioned method for estimating the distance to the desired foldpoint(s).

ii. *Methods for Computing Foldpoints.*

One of the central computational problems in connection with the equilibrium manifold M of a given

parametrized equation is the determination of the foldsets of M. These sets are of special importance in stability considerations for the equilibrium problems under study.

As mentioned in the previous sub-section, the availability of the simplicial meshes opens up a unique way of detecting the presence of such foldpoints. The points on the simplicial approximation also provide approximations for these foldpoints from where local iterative processes can be started for their accurate calculation. All such iterative methods require a suitably augmented system of equations for which the Jacobian is non-singular at the desired foldpoint. For some time now, the study of various classes of such augmenting schemes has been an active topic of research under this project. In particular, in [2] we consider augmentations of the form

$$F(x) = 0$$

$$c^T u_j = 0 \qquad j=1, \cdots, p$$

where the u_j form an orthonormal basis of the tangent space at the point x and c is a vector in the intersection of the normal space at that point with the parameter space Λ. This augmentation was shown to be feasible at singular points of socalled type (p,1,1) which includes the standard turning points, simple bifurcation points, and also various other types of singularities.

The crucial point in the utilization of this augmentation is the choice of the "unfolding" vector c. During the past year a new method has been developed to obtain such a vector c when x is an approximation of some foldpoint x* of the manifold [3]. The technique is closely related to the approach mentioned in the previous sub-section for estimating the distance $\|x-x^*\|$. A principal idea is the use of the so-called gap between the tangent space at x and the parameter space Λ. As part of this approach it has become possible to generate a new augmentation

$$F(x) = 0$$

$$g_j(x) = 0, \qquad j=1, \cdots, p$$

with the desirable property that the finite difference approximations of the derivatives of the g_j can be obtain directly from the Jacobian of F. Moreover, for paths of foldpoints this particular choice of the augmentation allows us to determine the approximate direction of a path of foldpoints on the manifold. With this we have

obtained a new method for continuing along such paths of foldpoints which turns out to be considerably more efficient than other methods known so far. More generally, the new augmentation has also opened up the possibility of determining the tangent directions of a higher dimensional sub-manifold of foldpoints. This, in turn, provides for the application of the simplicial approximation algorithm to such sub-manifolds. Such "triangulations" of foldsets have never been obtained before and they offer promising new approaches for the analysis of stability problems.

iii. *Error Estimations*

There are numerous error questions arising in the different processes for computing foldpoints on a solution manifold. During the past year we have begun a systematic study of the sources of these errors and of methods for estimating them. This work has addressed the following computational tasks related to the determination of foldpoints.

(a) *Detection problem:*

This important problem may be phrased as follows: Given a set $\{x^1, \ldots, x^k\}$ of points and appropriate additional information about the mapping at these points, determine whether some foldpoint of the manifold M is in a neighborhood of this set.

This is in essence a question of determining how far a given point is from a solution of a suitable augmented system of equations. Evidently, on the basis of information at finitely many points alone we cannot expect to obtain a guaranteed inclusion result; at least some information about the mapping in a suitable neighborhood of the given set of points is needed. This is already seen for very simple cases. Suppose that $\Lambda = span(v)$ and that x^1 and x^2 are two successive points produced by a continuation procedure. If both points belong to the same connected component of the continuation path and u^1 and u^2 are the corresponding (oriented) tangent vectors then $sgn(v^T u^1) \neq sgn(v^T u^2)$ implies that there is a limit point of odd order between these points. Evidently without further information about the mapping we cannot verify that both points belong to the same connected component of the path and without that assumption the statement need not hold. On the other hand, suppose that we only know that the two points are on the path and that we have oriented the tangent vectors by the requirement $(u^1)^T(u^2) > 0$. Now, it turns out that when a certain determinant changes sign

between the points and the points are not too far apart, then they cannot belong to the same connected component and hence there must be a bifurcation point between them.

These observations extend to the general case of a p-dimensional manifold. Once again the availability of a simplicial approximation of the manifold and of some derived quantities, as, for instance, an approximate curvature tensor, provides here some of the needed information for the development of methods for handling the detection problem.

(b) *Approximation error*

For a given approximation x of a foldpoint x* of M estimate the distance $||x-x^*||$ between these points. This depends on the measure of the distance between the points; at the same time some information about the mapping is needed to derive estimates of the distance. Here, as noted in subsection 1 above the size of the smallest principal angle between the m-dimensional normal space of the manifold at the point x and the p-dimensional natural parameter space Λ gives some information about this error. These principal angles are readily computed, but again information about the mapping is needed to derive from this an actual estimate of $||x-x^*||$. As mentioned earlier, an approximate value of the local curvature tensor proves very useful in this connection.

(c) *Foldpoint computation*

We have discussed already methods for the computation of specific foldpoints on our manifold. In all cases a suitably augmented system of equations is formed which then allows the application of a standard, locally convergent iterative process. The behavior of this process is controlled by the error of the initial approximation, the termination error of the method, and the influence of round-off on the reliability of the result. The initial approximation error was already discussed under (a) above. But the application of the iterative process provides some additional data which permit a closer estimation of that error. In connection with the termination error we are not only interested in the question how close the computed point is to the manifold, but how well it actually approximates the desired foldpoint. Thus we are again back to the previous problem. But once again, the behavior of the iterative process provides some information that was not available before and that appears to help in gaining a closer estimate.

References

1. P. J. Rabier and W. C. Rheinboldt, "On a Computational Method for the Second Fundamental Tensor and its Application to Bifurcation Problems", University of Pittsburgh, Institute for Computational Mathematics and Applications Technical Report ICMA-89-131. To appear in: *Numer. Math.*
2. J. P. Fink and W. C. Rheinboldt, "A Geometric Framework for the Numerical Study of Singular Points", University of Pittsburgh, Institute for Computational Mathematics and Applications Technical Report ICMA-86-90, 1986. *SIAM J. Num. Anal.*, 24, p. 618-633, 1987.
3. R.-X. Dai and W. C. Rheinboldt, "On the Computation of Manifolds of Foldpoints for Parameter-Dependent Problems", to appear *SIAM J. Numer. Anal.*

7. Differential Algebraic Equations (DAE'S) in Mechanics

Many problems in mechanics are of the generic form:

$$\underline{F}(\underline{x}) = 0 \tag{1}$$

$$A(\underline{x})\,\dot{\underline{x}} = \underline{G}(\underline{x}) \tag{2}$$

where $\underline{x} \equiv (\underline{z},\underline{\lambda})$, $\underline{z}$ is from a state space Z and $\underline{\lambda}$ is from a p dimensional parameter space Λ. Equation (1) is a set of nonlinear algebraic equations and (2) is a set of differential equations, hence the system (1)-(2) is termed a DAE.

An alternate interpretation comes from the observation that (1) defines a manifold M of dimensions p in the combined space $X = Z \times \Lambda$ and that (2) is a differential equation on M; hence the system (1)-(2) is also referred to as a *differential equation on a manifold* (DEM).

Two applications of interest to the investigators in which DEM's or DAE's occur are:

(i) *Incompressible Fluid Flow.* The continuity equation is an algebraic constraint of the form (1) and the time-dependent Navier-Stokes equation is a differential equation of the form (2).

(ii) *Punch Stetching of Sheet Metal.* The principle of virtual work provides a force equilibrium equation which defines an equilibrium manifold upon which one seeks solutions to differential constitutive laws of the form (2).

i. *Elastic-Plastic Deformation*

In [12], a new numerical method was presented for computer simulations of punch stretching of sheet metal. Most current approaches to finite element modeling of large deformation, elastic-plastic sheet metal forming use a rate form of the equilibrium equations and then must correct at each time step to insure that equilibrium is satisfied. Such methods are referred to as *incremental methods* [3]. The new method, a *DEM* approach discretizes the more fundamental equilibrium equations in non-rate form and insures equilibrium of forces at each time step. Formulating the problem as a DEM or DAE also allowed for solution of the discretized system using off-the-shelf software such as LSODI [14]. Numerical experimentation indicated that the DEM approach was, in many cases, computationally more efficient than the incremental approach.

Differential-algebraic systems (DAE's) are usually solved by means of software developed originally for the solution of initial value problems of ordinary differential equations (ODE's). This approach has become widely accepted ever since it was proposed by Gear [4]. Such codes as LSODI [14] and DASSL [15] are based on this approach in which the algebraic equations are viewed as degenerate ODE's.

An alternative approach is the DEM approach mentioned earlier, (see also [5]). The DAE is viewed as a differential equation on a manifold; the latter determined by the algebraic equations. Hence we seek a curve passing through the initial point whose tangent conforms to the direction field defined by the differential equations. This interpretation allows for the application of the differential- geometric techniques discussed in earlier sections. In particular, it suggests to new methods for the solution of DAE's especially in cases where the ODE methods no longer work very well.

Our experience in [12,13] gave strong indications that the DAE's arising in finite element discretizations of elasto-viscoplastic problems can not always be solved efficiently by ODE-software, such as LSODI. Problems appear to be related to the inability of the predictor to handle sudden changes in external forces due to punch or die contact, and to the onset of plasticity.

Computerized mathematical models which produce accurate and efficient simulations of sheet metal forming processes are highly useful for example in the automobile industry as a means of predicting the success or failure of a punch-die design, or evaluating formability properties of new materials. The differential equations on a manifold (DEM) method, coupled with state-of-the-art software packages designed to integrate differential

algebraic equations (DAE's), has proven to be such a model.

The basic equations governing the solution of large deformation plasticity problems in continuum mechanics are the equilibrium equations and the constitutive equations. In discretized form, the equilibrium conditions become a system of nonlinear algebraic equations, while the elastic-plastic constitutive equations are a system of ordinary differential equations (ODE's). Two general approaches to the solution of such differential-algebraic equations (DAE's) are typically used in displacement-based finite element methods. In one approach, the time derivative of the equilibrium equations is calculated and the DAE becomes an ODE in nodal displacements. In another, the equilibrium equation is left unchanged and during each time iteration of the nodal displacements, the constitutive equations are integrated to yield the stress, which is then used to check for equilibrium.

The Differential Equation on a Manifold (DEM) method as presented in [12] is similar to the latter approach in that the original equilibrium equations are used, however, as in the mixed methods the stresses as well as the displacements have finite element approximations. The equilibrium equations are viewed as a manifold in the solution space on which the solutions to the ODE (constitutive equations) must be traced. State-of-the-art numerical software is then used to solve the resulting DAE. Equilibrium is satisfied at each time step.

The DEM method was applied successfully to axisymmetric hydrostatic bulging [12] and to axisymmetric and plane strain sheet metal forming problems [13]. As compared to previous results [3], the DEM method produced accurate solutions for rate-sensitive materials for computational running times which range from 6 to 26 times less than for previous methods. The software package LSODI [14] was used for the numerical integration of the DAE's. These implementations of the DEM method for punch stretching resulted in an efficient and accurate, but somewhat non-robust algorithm.

In order to assess better the expected behavior of the solutions, a study of the existence and uniqueness of nonlinear DAEs was begun. In [21] such a theory was presented for first and second order systems of the form

$$F_1(x) = 0$$
$$F_2(x, x', z) = 0$$

and

$$F_1(x) = 0$$
$$F_2(x, x', x'', z) = 0 ,$$

respectively. For these systems it was shown that they induce smooth vector fields on certain open subsets of the space of their differentiable variables x. Moreover, in the first order case these vector fields are tangential to the constraint manifolds $\{x; F_1(x) = \text{constant}\}$ while for the second order equations they are tangential to the tangent bundles of these manifolds. This in turn provides directly for the desired existence and uniqueness of these DAEs. The theory has also opened up the development of a new local parametrization approach for the computational solution of these systems. This generalizes earlier developed techniques for the Euler-Lagrange equations arising in constrained multibody dynamics.

ii. *Bifurcation Phenomena*

Our computational experience with sheet-metal forming has also given strong indication that in the solution of DAE's there are situations in which singularities, such as bifurcations, occur. In particular, certain nonlinear DAE's may exhibit multiple solutions in some domains. Two examples of such a situation are the following:

(a) A geometrically symmetric plane strain punch problem, such as we considered in [12, 13], was modeled successfully using a natural symmetry. However, when this symmetry was ignored the solver (in this case LSODI) produced, what appeared to be, two distinct solution curves after the onset of plasticity depending on the particular problem parameters. One of these curves corresponded to the expected symmetric solution while the other one was clearly un-symmetric, which suggests the occurrence of a symmetry breaking bifurcation point.

(b) An extension of the DEM approach to in-plane stretching by Punch [6] led to a similar situation in which LSODI failed to follow a geometrically symmetric solution curve in favor of one which was non-symmetric.

These examples point to the necessity of a closer study of the singularities of DAE's. It appears that up to now very few results are available in this area.

The recent theoretical work [10], gives a complete and rigorous analysis of the dynamics in the vicinity of a generic singular point. The results in [10] explain why such deviations from the expected symmetric solution occur, which are due to the slightest breaking of a perfectly symmetric problem. Numerically, such a breaking

may be caused e.g. by roundoff. More interestingly, since actual problems are never perfectly symmetric, these results show that the true solution may well eventually lose symmetry completely, because the symmetric configuration becomes, loosely speaking, "unstable" beyond the singularity. This demonstrates that enforcing symmetry of the solution by reducing the size of the system, although tempting numerically, is not a safe procedure if a singularity is encountered, for then the calculated solution is no longer significant beyond the singularity. This phenomenon is largely (and probably totally) unknown and its discovery could have considerable importance in problems in which symmetry of the solution is routinely taken for granted because it is "obvious.". From now on, consideration should be given to the nonobvious and unsuspected fact that the slightest breaking of symmetry has drastic effects on the solution in fixed finite time.

In the case of the punch problem described in [13], a careful monitoring of the eigenvalues by Y. Huang, a Ph.D. student of Professors Hall and Rabier, has shown that, indeed, a singularity of the expected type is involved. This has been observed using various mesh sizes for the discretization and only little dependence on the critical time has been observed. A summary of these calculations with expanded comments is currently in preparation ([11]).

Of course, the understanding of the dynamics in the vicinity of generic ("standard" in the terminology of [10]) singular points of differential equations allows one to ask precise corresponding numerical questions, with a natural priority given to the development of reliable techniques for the characterization and computation of such points. One difficulty in this respect is that the approach taken in [10] is essentially theoretical and has no numerical counterpart. However, striking analogies between these standard singular points and the much more familiar turning points in transcendental equations make it plausible that appropriate variants of methods for the calculation of turning points exist, that can successfully be used for the determination of singular points.

The investigation of problems exhibiting symmetries has led, indirectly and unexpectedly, to new results in problems of bifurcation involving symmetry (see [20]) and having consequences in abstract group theory itself ([21]). These results also have important potential applications to the numerical treatment of such problems which are currently under study.

[1] M. Y. Lin Lee, "The Reduced Basis Method for Differential-Algebraic Systems", University of Pittsburgh, Institute for Computational Mathematics and Applications, Technical Report ICMA-85-85 (1985).

[2] T. A. Porsching and M. Lin Lee, "The Reduced Basis Method for Initial Value Problems", University of Pittsburgh, Institute for Computational Mathematics and Applications, Technical Report ICMA-86-95 (1986).

[3] N. M. Wang and M. L. Wenner, "Elastiviscoplastic analyses of simple stretch forming problems," *Proc. General Motors Research Laboratories Symposium*, New York, Plenum Press (1978).

[4] C. W. Gear, "Simultaneous Numerical Solution of Differential-Algebraic Equations", *IEEE Trans. on Circuit Theory*, CT-18 (1971) 89-95.

[5] W. C. Rheinboldt, "Differential-Algebraic Systems as Differential Equations on Manifolds", University of Pittsburgh, Institute for Computational Mathematics and Applications, Technical Report ICMA-83-55 (1983).

[6] E. F. Punch, "Plane Stretching Analysis Using the DEM Approach", GMR Research Dept. MA-340 (June, 1986).

[7] M. Roche, "Rosenbrock Methods for Differential Algebraic Equations", Ph D. Dissertation, Univ. de Geneva, Sept. 1986.

[8] P. J. Rabier and W. C. Rheinboldt, On a computational method for the second fundamental tensor and its applications to bifurcation problems, Technical Report ICMA-89-131 (to appear in *Numer. Math.).*

[9] P. J. Rabier and W. Rheinboldt (in preparation).

[10] P. J. Rabier, "Implicit differential equations near a singular point", *J. Math. Anal. Appl., 144*, pp. 425-449 (1989).

[11] C. A. Hall, Y. Huang and P. J. Rabier (in preparation).

[12] J. C. Cavendish, M. L. Wenner, J. Burkardt, C. A. Hall and W. C. Rheinboldt, "DEM: a new computational approach to sheet forming problems", *Int. J. Numer. Methods Eng.*, 23, 847-862.

[13] J. C. Cavendish, M. L. Wenner, J. Burkardt, C. A. Hall and W. C. Rheinboldt, "Punch Stretching of Sheet Metal and Differential Equations on Manifolds", *Int. J. Numer. Methods Engg.*, 25, (1988) 269-282.

[14] A. C. Hindmarsh, "ODE solvers for time-dependent PDE software", Presented at the IFIP PDE Software Conference, Soderkoping, Sweden, August 1983; available in preprint from as UCRL-89311, Lawrence Livermore National Laboratory.

[15] L. R. Petzold, "A description of DASSL: A differential/algebraic system solver", Proceedings of IMACS World Congress, Montreal, Canada, August 982.

[16] C. A. Hall, W. C. Rheinboldt and M. L. Wenner, "Differential equations on a manifold (DEM) formulations of metal forming", *NUMIFORM 89*, Proc. of Int. Conf. on Industrial Forming Processes, Balkema Publishers (1989).

[17] A. Chorin, *Math. Comp.* 23, (1969) 341-353.

[18] Temam, *Arch. Rat. Mech. Anal.* 33, (1969) 377-385.

[19] Hundsdorfer, Report NM-R8708, Centre for Mathematics and Computer Science, Amsterdam.

[20] P. J. Rabier, "New aspects in bifurcation with symmetry", to appear in *Diff. Int. Eqs.*

[21] P. J. Rabier, "Intrinsic isotropy subgroups of finite groups", submitted to *J. of Algebra.*

[22] W. C. Rheinboldt, "A General Existence and Uniqueness Theorem for Implicit Differential-Algebraic Equations", Technical Reports ICMA-90-145, January 1990.

8. Bifurcation Theory and Singular ODE's.

In connection with differential algebraic equations (DAE's), a theoretical analysis of singular differential equations has been started in [5]. The problem is to determine the structure of the set of solutions to an initial value problem

$$\begin{cases} A(x)\dot{x} = G(x), \\ x(t_0) = x_0, \end{cases} \tag{1}$$

when the $n \times n$ matrix $A(x)$ is singular at $x = x_0$. The above formulation is suitable for the analysis of singularities occurring in DAE's as well, a framework in which the problem has received a great deal of attention from singular perturbation theory specialists. The approach taken in [5] follows ideas of bifurcation theory and has permitted, apparently for the first time, to eliminate the usual but restrictive assumption that $A(x)$ is singular on an entire neighborhood of x_0.

In actual applications, equation (1) generally does not exhibit a singularity at the beginning of evolution. However, it is quite possible that singularities appear at some later time along a trajectory. To describe what happens next, one must analyze problems of the form (1) with singular $A(x_0)$. As is shown in [5], existence of a singularity along a trajectory is not affected by small perturbations of the (nonsingular) initial condition: it is a stable and hence important phenomenon.

Our recent work on singular differential equations has followed two directions. First, we have derived reliable algorithms for the calculation of the singular points called "standard" in [4]. These points are of primary interest because, according to [5], most singular points are of this type in the generic case.

Starting with a problem of the form (1) with nonsingular $A(x_o)$, we assume existence of an unknown time $t_* > 0$ such that $A(x(t_*))$ is singular and propose methods for calculating t_* and $x_* \equiv x(t_*)$ in the assumption that x_* is a standard singular point.

The need for such methods can be hinted from the fact that the simple approach consisting in writing (1) in the explicit form

$$\begin{cases} \dot{x} = A^{-1}(x)G(x), \\ x(0) = x_0 \end{cases},$$

although legitimate for $t \in [0, t_*)$, leads to a problem in which the matrix $A(x(t))$ becomes singular as t approaches t_*. This, of course, may result in inaccuracies in the numerical calculation of both t_* and $x_* = x(t_*)$. It is important to point out that the singularity *cannot* be jumped over. Indeed, the analysis in [5] reveals that a trajectory encountering a standard singular point must necessarily terminate at the point: the solution $x(t)$ *cannot* be extended continuously for $t > t_*$. As far as numerical aspects are concerned, this forces the matrix $A(x(t))$ to remain in a state of quasi-singularity without possible escape as t approaches or exceeds t_* (numerically, t may exceed t_* despite the fact that this is theoretically impossible). This emphasizes the importance of having ad-hoc algorithms for the accurate calculation of standard singular points.

Such algorithms have been developed, which reduce the problem to solving a nonsingular ODE and scalar algebraic equations. Part of the procedure uses a variant of a minimal augmentation technique introduced by Griewank and Reddien [2] and extended by Rabier and Reddien [4], in connection with calculation of singularities in bifurcation problems. The possibility of modifying methods of numerical bifurcation theory to handle singular differential equations was anticipated in the previous research proposal. A related report [6] is currently being prepared.

The second component of the work recently accomplished in the domain of singular differential equations deals with their relevance in real life problems. Some of the authors of this proposal had been suspecting for a while that numerical inconsistencies observed in a problem of metal punching (see [1]) were due to the presence of a singularity. This has now been fully corroborated by numerical calculations based on the previously mentioned algorithms for the calculation of singular points. A report by Hall, Huang and Rabier ([3]) on this problem, and its importance and implications, is in preparation. Figure 1 illustrates the behavior of λ, the smallest eigenvalue (in modulus) of the Jacobian of the DAE (differential algebraic equation) resulting from the DEM modelling of a symmetric punch stretching of sheet metal problem described in [1]. As λ tends to zero in the vicinity of 28 secs, the numerical solution loses symmetry. It has been verified numerically, that the purely symmetric problem in fact has a Jacobian which is singular near this value of time. (See [3] for more details.). For various finite element meshes behavior is qualitatively similar.

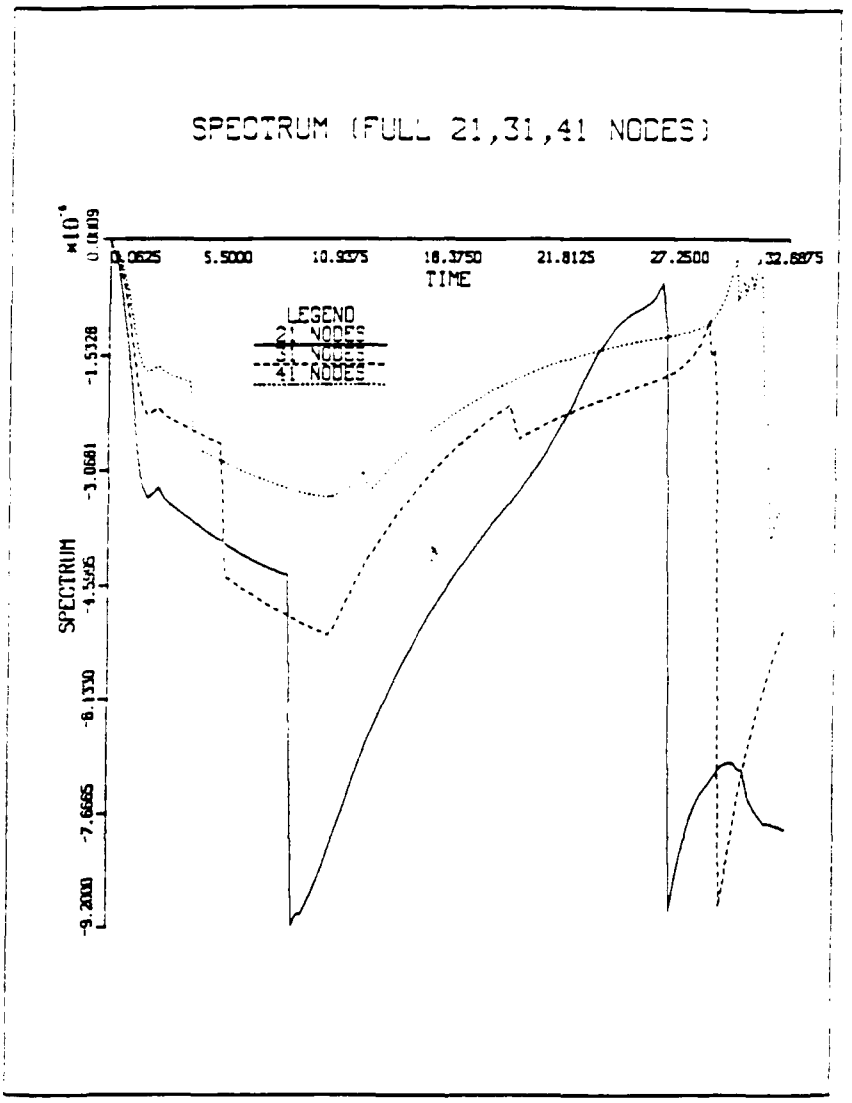

Figure 1.

References

[1] Cavendish, J. C., Wenner, M. L., Burkardt, J., Hall, C. A. and Rheinboldt, W. C., "Punch Stretching of Sheet Metal and Differential Equations on Manifolds", *Int. J. Num. Meth. Eng.*, 25, pp. 269-282 (1988)

[2] Griewank, A. and Reddien, G., "Characterization and computation of generalized turning points," *SIAM J. Num. Anal.*, *21*, pp. 176-185 (1984).

[3] Hall, C. A., Huang, Y. and Rabier, P. J., in preparation.

[4] Rabier, P. J. and Reddien, G., "Characterization and computation of singular points with maximum rank deficiency", *SIAM J. Num. Anal.*, *23*, pp. 1040-1051 (1986).

[5] Rabier, P. J., "Implicit Differential Equations Near a Singular Point", *J. Math. Anal. Appl.*, *144*, pp. 425-449 (1989).

[6] Rabier, P. J., in preparation.

II. PUBLICATIONS SUPPORTED BY AFOSR-88-0262

1. "Generic Aspects of Convexification with Applications to Thermodynamics Equilibrium", P. J. Rabier and A. Griewank, ICMA-88-129 (To appear in *Archive Rat. Mech. Anal.)*
2. "The Determination Modes Question for Nonlinear Operator Equations", J. Boland and W. Layton, ICMA-88-119.
3. "Differential Equations on a Manifold (DEM) Formulations of Metal Forming", C. A. Hall, W. C. Rheinboldt and M. L. Wenner, *Proceedings of the Int Conf. on Num. Meth. in Industrial Forming Processes,* June, 1989, Balkema Publishers, Rotterdam.
4. "Topological Degree and the Theorem of Borsuk for General Convariant Mappings", P. J. Rabier, ICMA-89-132. Submitted to *Nonlinear Analysis, TMA.*
5. "Approximation Methods in the Computer Numerically Controlled Fabrication of Optical Surfaces, Part 1: Finite Dimensional Material Removal Profile Spaces", C. A. Hall and T. A. Porsching, ICMA-89-134. Submitted to: *I.M.A.J.N.A.*
6. "Iterative Solution of Navier-Stokes Dual Variable Difference Equations", G. Mesina and C. A. Hall, ICMA-89-135, Submitted to: *J. Comp. Phys.*
7. "Construction of Divergence-Free Spaces for Incompressible Navier-Stokes Equations", Xiu Ye, Ph.D. Dissertation (Expected completion: August 1990.)
8. "New Aspects in Bifurcation with Symmetry", P. J. Rabier, To appear in *Diff. Int. Eqs.*
9. "Analytical and Numerical Studies of Natural Convection Problems", J. Boland, G. B. Ermentrout, C. A. Hall, W. Layton and H. Melhem, in: *Proc. Int. Conf. on Thy. and Appls. of Diff. Eqns.*, Athens, Ohio, 1988.
10. "Optimal Interior Estimates for the Defect-Correction, Finite Element Approach to 2-D Convection - Diffusion Problems", O. Axelsson and W. Layton, ICMA-88-116, to appear in: *R.A.I.R.O., J. Numer. Anal.*
11. "On the Principal Axes of Diffusion in Difference Schemes for 2-D Transport Problems", W. Layton, ICMA Report 88-124, *J. Comp. Phys.*, to appear.
12. "Analysis of the Finite Element Method for Natural Convection Problems", J. Boland and W. Layton, ICMA Report 88-126, *Num. Methods for PDE's.*, to appear.
13. "A Novel Monotone Type Difference Scheme for General, Second Order Elliptic Equations", W. Layton, K.U.N. Report, May 1989, submitted to: *Linear Alg. Appls.*
14. "On the Construction of Monotone Type Difference Stencils for Boundary Value Problems for Partial Differential Equations", W. Layton, submitted to *SIAM J. Alg. Disc. Methods.*
15. "Finite Element Methods for Steady Natural Convection Problems", J. Boland and W. Layton, submitted, currently under review.
16. "A Note on Contraction Numbers for Additive Correction Methods", S. H. Chou and T. A. Porsching, *Appl. Math. Lett.* 2 (1989), 83-86.
17. "Contraction Numbers for Additive Correction Methods", S. H. Chou and T. A. Porsching, To appear in *Linear Alg. Appls.*
18. "A Projected Bi-Conjugate Gradient Approach to Solving Discretized Incompressible Navier-Stokes Eqations", S. Choudhury, ICMA Report.
19. "Discretization of Incompressible Vorticity-Velocity Equations on Triangular Meshes", S. Choudhury and R. A. Nicolaides, to appear in *Int. J. Num. Meth. Fluids.*
20. "Iterative Methods as Discretization Procedures", O. Axelsson and W. Layton, to appear in: *Proc. Int. Conf. on P.C.G. and Appls.*, 1989.

III. PERSONNEL

Faculty

1. Shenaz Choudhury
   Assistant Professor of Mathematics

2. Charles A. Hall
   Professor of Mathematics

3. William J. Layton
   Associate Professor of Mathematics

4. Patrick Rabier
   Associate Professor of Mathematics

5. Thomas Porsching
   Professor of Mathematics

6. Mahlon Raymund
   Senior Lecturer

7. Werner C. Rheinboldt
   Andrew W. Mellon Professor of Mathematics

Graduate Research Assistants

Monica Brodzik
Leonard DeCarlo
Bin Hong
Yiping Huang
George Mesina
Victoria Radel
Xiu Ye